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XAS of Nucleophilic Zinc Enzymes

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Beamline(s): X9B

Epoxypropane: CoM transferase (Component 1 of the epoxide carboxylase system), catalyzes epoxide ring opening in the metabolism of small alkenes (propylene, in the case of Xanthobacter strain Py2). The enzyme contains a zinc site that has been suggested to be important in catalysis. EXAFS spectroscopy has been used to determine the structure of the zinc site in epoxypropane: CoM transferase (C1) from *E. Coli* . In the absence of substrate the zinc has $ZnS_2(N/O)_2$ ligation, consistent with predictions based on sequence alignments of C1 with colbalamin-independent methionine synthase (MetE) from *E. Coli* and MT2: CoM methyltransferase (MT2) from *M. barkeri.* Addition of the CoM substrate to either the recombinant C1 or native C1 converted the zinc site to a $ZnS_3(N/O)$ site. Addition of epoxypropane to C1 + CoM returns the Zn to $ZnS_2(N/O)_2$ ligation. However, both the EXAFS and the XANES data demonstrate that the Zn site in C1 + CoM + epoxypropane is distinct from that in C1.